Chemistry is the study of matter and the changes material substances undergo.

It is essential for understanding much of the natural world and central to many other scientific disciplines, including astronomy, geology, paleontology, biology, and medicine.

Stoichiometry: Chemical Formulas and Equations

Chemists study the structures, physical properties, and chemical properties of material substances. These consist of matter, which is anything that occupies space and has mass.

What happens to matter when it undergoes chemical changes?

The law of conservation of mass:

Atoms are neither created, nor distroyed, during any chemical reaction

Thus, the same collection of atoms is present after a reaction as before the reaction. The changes that occur during a reaction just involve the *rearrangement* of atoms.

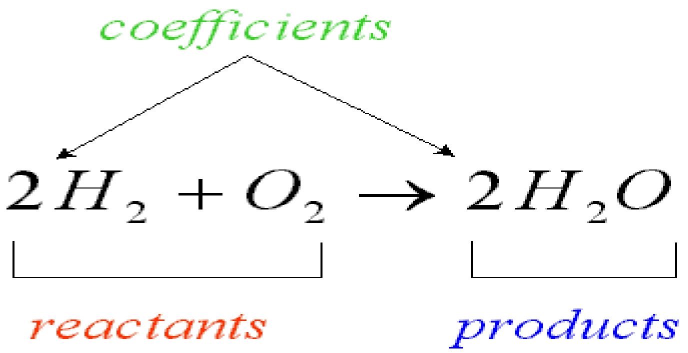
In this section we will discuss *stoichiometry* (the "measurement of elements").

Chemical equations

Chemical reactions are represented on paper by *chemical equations*. For example, hydrogen gas (H_2) can react (burn) with oxygen gas (O_2) to form water (H_20). The *chemical equation* for this *reaction* is written as:

$$2H_2 + O_2 \rightarrow 2H_2O$$

The '+' is read as 'reacts with' and the arrow '' means 'produces'. The chemical formulas on the left represent the starting substances, called reactants. The substances produced by the reaction are shown on the right, and are called products. The numbers in front of the formulas are called coefficients (the number '1' is usually omitted).



Because atoms are neither created nor destroyed in a reaction, *a chemical equation must have an equal number of atoms of each element on each side of the arrow* (i.e. the equation is said to be 'balanced').

$$2H_2 + O_2 \rightarrow 2H_2O$$

$$\begin{array}{ccccc} \downarrow & & \downarrow & & \downarrow \\ 4H, & & 2O & = & 4H,\ 2O \end{array}$$

Steps involved in writing a 'balanced' equation for a chemical reaction:

1. **Experimentally determine reactants and products**
2. **Write 'un-balanced' equation using formulas of reactants and products**
3. **Write 'balanced' equation by determining coefficients that provide equal numbers of each type of atom on each side of the equation (generally, whole number values)**

Note! Subscripts should never be changed when trying to balance a chemical equation. Changing a subscript changes the actual identity of a product or reactant. Balancing a chemical equation only involves changing the relative amounts of each product or reactant.

Consider the reaction of burning the gas methane (CH_4) in air. We know experimentally that this reaction consumes oxygen (O_2) and produces water (H_2O) and carbon dioxide (CO_2).

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

Now lets count up the atoms in the reactants and products:

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

$$\begin{array}{ccc} C=1 & & C=1 \\ H=4 & \neq & H=2 \\ O=2 & & O=3 \end{array}$$

Note that while this has balanced our carbon and hydrogen atoms, we now have 4 oxygen atoms in our products, and only have 2 in our reactants. We can balance our oxygen atoms by doubling the number of oxygen atoms in our reactants:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$\begin{array}{ccc} C=1 & & C=1 \\ H=4 & = & H=4 \\ O=4 & & O=4 \end{array}$$

We now have fulfilled step #3, we have a *balance chemical equation* for the reaction of methane with oxygen. Thus, *one molecule of methane reacts with two molecules of oxygen to produce one molecule of carbon dioxide and two molecules of water*.

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$$

<u>Stoichiometry: Patterns of Chemical Reactivity</u>

We can often predict a reaction if we have seen a similar reaction before. For example, sodium (Na) reacts with water (H_20) to form sodium hydroxide (NaOH) and H_2 gas:

$$2Na(s) + 2H_2O(l) \rightarrow 2NaOH(aq) + H_2(g)$$

note: (aq) indicates aqueous liquid

Combustion in air

***Combustion reactions are rapid reactions that produce a flame*. Most common combustion reactions involve oxygen (O_2) from the air as a *reactant*. A common class of compounds which can participate in combustion reactions are *hydrocarbons* (compounds that contain only carbon and hydrogen).**

Examples of common hydrocarbons:

Name	Molecular formula
methane	CH_4
propane	C_3H_8
butane	C_4H_{10}
octane	C_8H_{18}

When hydrocarbons are combusted they react with oxygen (O2) to form carbon dioxide (CO_2) and water (H_2O). For example, when propane is burned the reaction is:

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$

Other compounds which contain carbon, hydrogen and oxygen (e.g. the alcohol *methanol* CH_3OH, and the sugar *glucose* $C_6H_{12}O_6$) also combust in the presence of oxygen (O_2) to produce CO_2 and H_2O.

Combination and decomposition reactions

In *combination reactions* two or more compounds react to form *one* product:

$$A + B \rightarrow C$$

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

In *decomposition reactions* one substance undergoes a reaction to form two or more products. For example, many metal carbonates undergo a heat dependent decomposition to the corresponding oxide plus CO_2:

$$A \rightarrow B + C$$

$$\underbrace{CaCO_3(s)}_{\text{limestone}} \xrightarrow{Heat} \underbrace{CaO(s)}_{\text{`quicklime'}} + CO_2(g)$$

Stoichiometry: Atomic and Molecular Weights

The subscripts in chemical formulas, and the coefficients in chemical equations represent *exact* quantities.

H_2O, for example, indicates that a water molecule comprises exactly two atoms of hydrogen and one atom of oxygen.

The following equation:

$$C_3H_8(g) + 5O_2(g) \longrightarrow 3CO_2(g) + 4H_2O(l)$$

not only tells us that propane reacts with oxygen to produce carbon dioxide and water, but that *1* molecule of propane reacts with *5* molecules of oxygen to produce *3* molecules of carbon dioxide and *4* molecules of water.

Since counting individual atoms or molecules is a little difficult, quantitative aspects of chemistry rely on knowing the *masses* of the compounds involved.

The atomic mass scale

***Atoms of different elements have different masses*. Early work on the separation of water into its constituent elements (hydrogen and oxygen) indicated that 100 grams of water contained 11.1 grams of hydrogen and 88.9 grams of oxygen:**

100 grams Water -> 11.1 grams Hydrogen + 88.9 grams Oxygen

Later, scientists discovered that water was composed of *two atoms* of hydrogen *for each atom* of oxygen. Therefore, in the above analysis, *in the 11.1 grams of hydrogen there were twice as many atoms as in the 88.9 grams of oxygen.*

Therefore, an oxygen atom must weigh about 16 times as much as a hydrogen atom:

$$\left(\left(\frac{88.9\text{g Oxygen}}{1\text{ atom}}\right) \Big/ \left(\frac{11.1\text{g Hydrogen}}{2\text{ atoms}}\right)\right) = 16$$

Hydrogen, the lightest element, was assigned a relative mass of '1', and the other elements were assigned 'atomic masses' relative to this value for hydrogen. Thus, oxygen was assigned an atomic mass of 16.

We now know that a hydrogen atom has a mass of 1.6735×10^{-24} grams, and that the oxygen atom has a mass of 2.6561×10^{-23} grams. As we saw earlier, it is convenient to use a reference unit when dealing with such small numbers: the atomic mass unit. The atomic mass unit (*amu*) was not standardized against hydrogen, but rather, against the ^{12}C isotope of carbon (*amu* = 12).

Thus, the mass of the hydrogen atom (^{1}H) is 1.0080 *amu*, and the mass of an oxygen atom (^{16}O) is 15.995 *amu*. Once the masses of atoms were determined, the *amu* could be assigned an actual value:

$$1\ amu = 1.66054 \times 10^{-24}\text{ grams}$$

conversely:

$$1\text{ gram} = 6.02214 \times 10^{23}\ amu$$

Average atomic mass

Most elements occur in nature as a mixture of *isotopes* (i.e. populations of atoms with different numbers of neutrons, and therefore, mass). We can calculate the average atomic mass of an element by knowing the relative abundance of each isotope, as well as the mass of each isotope.

Example: Naturally occurring carbon is 98.892% ^{12}C and 1.108% ^{13}C. The mass of ^{12}C is 12 amu, and that of ^{13}C is 13.00335 amu. Therefore, the *average atomic mass of carbon is:*

$$(0.98892)*(12\ amu) + (0.01108)*(13.00335\ amu) = 12.011\ amu$$

The average atomic mass of each element (in amu) is also referred to as its *atomic weight*. Values for the atomic weights of each of the elements are commonly listed in periodic tables.

Formula and Molecular Weights

***The formula weight of a substance is the sum of the atomic weights of each atom in its chemical formula*.**

For example, water (H_2O) has a formula weight of:

$$2*(1.0079\ amu) + 1*(15.9994\ amu) = 18.01528\ amu$$

If a substance exists as discrete molecules (as with atoms that are *chemically bonded* together) then the *chemical formula* is the *molecular formula*, and the *formula weight* is the *molecular weight*. For example, carbon, hydrogen and oxygen can chemically bond to form a molecule of the sugar glucose with the chemical and molecular formula of $C_6H_{12}O_6$. The formula weight and the molecular weight of glucose is thus:

$$6*(12\ amu) + 12*(1.00794\ amu) + 6*(15.9994\ amu)$$
$$= 180.0\ amu$$

Ionic substances are not chemically bonded and do not exist as discrete molecules. However, they do associate in discrete ratios of ions. Thus, we can describe their formula weights, but not their *molecular weights*. Table salt (NaCl), for example, has a formula weight of:

$$23.0\ amu + 35.5\ amu$$
$$= 58.5\ amu$$

Percentage composition from formulas

In some types of analyses of it is important to know the *percentage by mass* of each type of element in a compound. Take for example methane:

$$CH_4$$

Formula* and *molecular* weight: 1*(12.011 *amu*) + 4*(1.008) = 16.043 *amu

$$\%C = 1*(12.011\ amu)/16.043\ amu = 0.749 = 74.9\%$$
$$\%H = 4*(1.008\ amu)/16.043\ amu = 0.251 = 25.1\%$$

Stoichiometry: Chemical Formulas and Equations

Limiting reactants

Suppose you are a chef preparing a breakfast for a group of people, and are planning to cook French toast. You make French toast the way you have always made it: one egg for every three slices of toast. You never waiver from this recipe, because the French toast will turn out to be either too soggy or too dry (arguably, you are anal retentive). There are 8 eggs and 30 slices of bread in the pantry. Thus, you conclude that you will be able to make 24 slices of French toast and not one slice more.

This is a similar situation with chemical reactions in which one of the reactants is used up before the others - the reaction stops as soon as one of the reactants is consumed. For example, in the production of water from hydrogen and oxygen gas suppose we have 10 moles of H_2 and 7 moles of O_2.

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$$

Because the *stoichiometry* of the reaction is such that 1 mol of O_2 $\hat{=}$ 2 moles of H_2, the number of moles of O_2 needed to react with all of the H_2 is:

$$\left(\frac{1 mole O_2}{2 moles H_2}\right) * 10 moles H_2 = 5 moles O_2$$

Thus, after all the hydrogen reactant has been consumed, there will be 2 moles of O_2 reactant left.

The reactant that is completely consumed in a chemical reaction is called the limiting reactant (or limiting reagent) because it determines (or limits) the amount of product formed.

In the example above, the H_2 is the limiting reactant, and because the stoichiometry is $2H_2$ $\hat{=}$ $2H_2O$ (i.e. H_2 $\hat{=}$ H_2O), it limits the amount of product formed (H_2O) to 10 moles.

We actually have enough oxygen (O_2) to form 14 moles of H_2O ($1O_2$ $\hat{=}$ $2H_2O$).

One approach to solving the question of which reactant is the limiting reactant (given an initial amount for each reactant) is to calculate the amount of product that could be formed from each amount of reactant, assuming all other reactants are available in unlimited quantities. In this case, the limiting reactant will be the one that produces the least amount of potential product.

Consider the following reaction:

$$2Na_3PO_4(aq) + 3Ba(NO_3)_2(aq) \rightarrow Ba_3(PO_4)_2(s) + 6NaNO_3(aq)$$

Suppose that a solution containing 3.50 grams of Na_3PO_4 is mixed with a solution containing 6.40 grams of $Ba(NO_3)_2$. How many grams of $Ba_3(PO_4)_2$ can be formed?
